Generalized Procrustes Analysis

The following notes on generalized Procrustes Analysis are based on: I. Borg and Patrick J. F. Groenen, Modern Multidimensional Scaling (2nd ed.) (Springer, NY, 2005).

While scaling and translation are complicated (indeed, they are complicated for any non-orthogonal transformation), in `Procrustes` we've elected to use a simple scaling/translation methodology. So we will assume that the input matrices, $\mathbf{A}_k$ are scaled and translated by the normal rules, if that is desired.

The objective function is obtained by transforming multiple matrices in generalized Procrustes analysis. So:

$$\underbrace{\min}_{\mathbf{T}_1,\mathbf{T}_2,\ldots\mathbf{T}_K} \sum_{1\leq k<l\leq N} \left\|\mathbf{A}_k\mathbf{T}_k - \mathbf{A}_l\mathbf{T}_l\right\|^2 = \underbrace{\min}_{\mathbf{T}_1,\mathbf{T}_2,\ldots\mathbf{T}_K} \sum_{1\leq k<l\leq N} \text{Tr}\left[\left(\mathbf{A}_k\mathbf{T}_k - \mathbf{A}_l\mathbf{T}_l\right)^\dagger \left(\mathbf{A}_k\mathbf{T}_k - \mathbf{A}_l\mathbf{T}_l\right)\right]$$

can be solved by rewriting this as

$$\underbrace{\min}_{\mathbf{T}_1,\mathbf{T}_2,\ldots\mathbf{T}_K} \frac{1}{2}\left\|\sum_{1\leq k\leq K}\left(\mathbf{A}_k\mathbf{T}_k - \sum_{\substack{1\leq l\leq N\\ l\neq k}}\mathbf{A}_l\mathbf{T}_l\right)\right\|^2$$

Then you can decide to optimize this expression either by reference to the mean of the matrices or by optimizing one transformation at a time. The former is arguably easier to implement (and generalize), though it isn't what we are doing right now. In that case, for each $k = 1, 2, \ldots, K$, one solves the single-matrix Procrustes problem,

$$\underbrace{\min}_{\mathbf{T}_k}\left\|\left(\mathbf{A}_k\mathbf{T}_k^{(i)} - \sum_{\substack{1\leq l\leq N\\ l\neq k}}\mathbf{A}_l\mathbf{T}_l^{(i-1)}\right)\right\|^2$$

where it is sensible (but not required) to initialize the transformations to the identity, $\mathbf{T}_k^{(0)} = \mathbf{I}$. As long as the optimization is linear, this algorithm converges, and is equivalent to the usual approach.

The nice thing about this algorithm is that it generalizes to *any* generalized Procrustes problem. If you pass multple matrices to any Procrustes method, then you end up with the generic problem

$$\underbrace{\min}_{\substack{\mathbf{T}_1,\mathbf{T}_2,\ldots\mathbf{T}_K\\ \mathbf{S}_1,\mathbf{S}_2,\ldots\mathbf{S}_K}} \sum_{1\leq k<l\leq N}\left\|\mathbf{S}_k\mathbf{A}_k\mathbf{T}_k - \mathbf{S}_l\mathbf{A}_l\mathbf{T}_l\right\|^2$$

which can be (approximately) solved by iteratively performing, for $k = 1, 2, \ldots, K$,

$$\underbrace{\min}_{\mathbf{T}_k} \left\| \left(\mathbf{S}_l^{(i)} \mathbf{A}_k \mathbf{T}_k^{(i)} - \sum_{\substack{1 \leq l \leq N \\ l \neq k}} \mathbf{S}_l^{(i-1)} \mathbf{A}_l \mathbf{T}_l^{(i-1)} \right) \right\|^2$$

until it converges.